

A quantum resonance catastrophe for transport through an AC driven impurity

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We consider the quantum transport in a tight-binding chain with a locally applied potential which is oscillating in time. The steady state for such a driven impurity can be calculated exactly for any energy and applied potential using the Floquet formalism. The resulting transmission has a non-trivial, non-monotonic behavior depending on incoming momentum, driving frequency, and the strength of the applied periodic potential. Hence there is an abundance of tuning possibilities, which allows to find resonances of total reflection for any choice of incoming momentum and periodic potential. Remarkably, this implies that even for an arbitrarily small infinitesimal impurity potential it is always possible to find a resonance frequency at which there is a catastrophic breakdown of the transmission $T = 0$. The points of zero transmission are closely related to the phenomenon of Fano resonances at dynamically created bound states in the continuum. The results are relevant for a variety of one-dimensional systems where local AC driving is possible, such as quantum nanodot arrays, ultracold gases in optical lattices, photonic crystals, or molecular electronics.

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Driven quantum systems appear in many different contexts in physics and chemistry [1–10]. At the same time there has been remarkable progress in the controlled design of nanoscale quantum systems with a high degree of coherence and tunability. Systems containing just a few molecules are promising candidates for the realization of electronic components on the sub-silicon scale (molecular electronics) [11–16]. The quantum transfer of particles between such localized structures can be well described by the tight-binding model in order to gain understanding of the transport mechanisms involved [17–20]. Another versatile realization of near-perfect tight-binding models are ultracold gases in optical lattices with a great variety of possible geometries [21], where tunable local impurities [22], periodic driving [6–10], and dimensional crossover [23] have also been realized. Tight-binding models are also applicable when investigating other driven systems such as quantum dot arrays [3]. Finally, photonic cavities and photonic crystals have been used as quantum simulators to fabricate interesting quantum tight-binding systems [24–26]. In practical applications time-dependent effects such as electromagnetic radiation or gate voltages can be used to manipulate the transport properties of nanodevices [3]. Driven tunneling between two quantum wells has been well studied [3–6]. A natural further development is the transport through a driven impurity in an extended structure of coupled wells with a finite bandwidth.

In the present Letter we consider the steady state of a generic model system, consisting of a one-dimensional tight-binding chain for bosons or fermions with a periodically varying potential μ at one impurity site ($i = 0$)

$$H = -J \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) - \mu \cos(\omega t) c_0^\dagger c_0, \quad (1)$$

where we have used standard notation and the hopping

amplitude is denoted by J . This model captures the essential physics of a single one-dimensional band, which is useful for the description of corresponding AC driven experimental setups mentioned above. Higher energy bands may give interesting additional effects at very high frequencies, but this will not change the central results in this work since the most interesting physics turns out to involve excitations close to the band-edge.

It is well-known that for a static barrier, the phenomenon of tunneling allows transport for any finite potential strength μ . In strong contrast, the time-periodic potential considered here turns out to show resonances at special driving frequencies where the transmission is completely blocked. In fact, we will show that it is always possible to find such a finite resonance frequency ω for any combination of incoming momentum k and barrier strength μ . This implies that even for an *infinitesimally small* periodic perturbation μ there is a complete breakdown of conductance, if the frequency ω is tuned to the corresponding resonance. We call this phenomenon the *quantum resonance catastrophe*.

The goal of this paper is to calculate the transport of an incoming particle with a given momentum k and corresponding energy $\epsilon = -2J \cos k$, which is the dispersion relation of the model in Eq. (1) away from the impurity. Just like in the static case, the transmission coefficient can be determined from the steady state solution of the Schrödinger equation $(H(t) - i\partial_t)|\Psi(t)\rangle = 0$. Due to the periodicity of the Hamiltonian $H(t) = H(t + 2\pi/\omega)$ it is possible to use the Floquet formalism [2, 27] to express any steady state solution in terms of so-called Floquet states $|\Psi(t)\rangle = e^{-i\epsilon t/\hbar} |\Phi(t)\rangle$, where ϵ is the quasi-energy of the resulting $(d+1)$ -dimensional eigenvalue equation $(H - i\partial_t)|\Phi(t)\rangle = \epsilon|\Phi(t)\rangle$ and the Floquet modes $|\Phi(t)\rangle = |\Phi(t + 2\pi/\omega)\rangle$ are periodic in time.

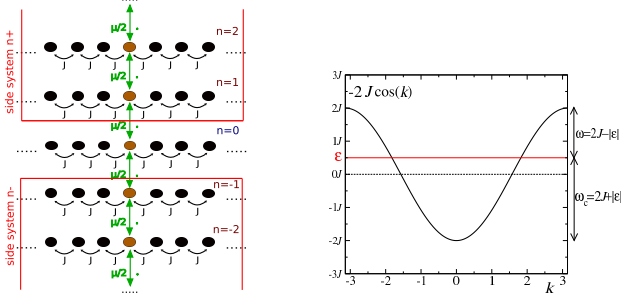


FIG. 1: *Left:* Sketch of the model mapped onto a set of static coupled chains. The $n = 0$ chain is locally connected to two side-coupled systems of chains with a corresponding chemical potential $n\omega$. *Right:* Dispersion relation with the special frequencies $\omega = 2J \pm \epsilon$ below which the side coupled chains $n = \mp 1$ start support unbound solutions for the case $\epsilon = 0.5J$.

Using the spectral decomposition

$$|\Phi(t)\rangle = \sum_{n=-\infty}^{\infty} e^{-in\omega t} |\Phi_n\rangle, \quad (2)$$

the eigenvalue equation for a Hamiltonian of the form $H(t) = H_0 + 2H_1 \cos(\omega t)$ becomes discrete in the time direction

$$H_0|\Phi_n\rangle + H_1(|\Phi_{n+1}\rangle + |\Phi_{n-1}\rangle) = (\epsilon + n\omega)|\Phi_n\rangle. \quad (3)$$

A general steady state on the tight-binding lattice is given by

$$|\Phi_n\rangle = \sum_j \phi_{j,n} c_j^\dagger |0\rangle. \quad (4)$$

The model in Eq. (1) therefore results in the following set of coupled equations

$$\begin{aligned} -J(\phi_{-1,n} + \phi_{1,n}) - \frac{\mu}{2}(\phi_{0,n+1} + \phi_{0,n-1}) &= (\epsilon + n\omega)\phi_{0,n} \\ -J(\phi_{j-1,n} + \phi_{j+1,n}) &= (\epsilon + n\omega)\phi_{j,n} \quad \text{for } j \neq 0 \end{aligned} \quad (5)$$

which effectively corresponds to a static Hamiltonian with eigenvalue ϵ for an infinite number of chains labeled by n , each with additional overall chemical potential of $n\omega$, analogous to a Wannier-Stark ladder [2]. The chains are coupled to each other only at site $j = 0$ by a hopping term $\mu/2$ as depicted in Fig. 1 (left). Notice that the entire problem is symmetric under parity transformation $j \rightarrow -j$, so that solutions are either parity symmetric or parity antisymmetric. The parity anti-symmetric solutions obey $\phi_{0,n} = 0$, $\forall n$, so they do not couple to the driving potential and can be ignored.

Transmission coefficient.— We now want to calculate the transmission of an incoming particle with momentum k and $\epsilon = -2J \cos k$ for the chain $n = 0$. The parity symmetric solution is given by plane waves of the general form

$$\phi_{j,0} = A \cos(|j|k - \theta). \quad (6)$$

Since the potential μ only affects a single impurity site for all chains, the solutions for $j \neq 0$ must correspond to wave-like states (unbound solutions) for $|\epsilon + n\omega| < 2J$ and bound states otherwise according to Eq. (5). As indicated in Fig. 1 (right) a critical frequency can be defined

$$\omega_c \equiv 2J + |\epsilon|. \quad (7)$$

For $\omega > \omega_c$ all chains with $n \neq 0$ are outside the band $|\epsilon + n\omega| > 2J$ and correspond to bound states. Below the frequency $\omega = \omega_c$ the first side coupled chain starts to support unbound solutions. A second unbound solution starts to appear below $\omega = 2J - |\epsilon|$ and so on.

Let us first consider frequencies $\omega > \omega_c$ with bound states for all $n \neq 0$ of the form

$$\phi_{j,n} = C_n e^{-\kappa_n |j|} \text{sign}(-n)^{j+n}, \quad (8)$$

where $\epsilon + n\omega = 2J \text{sign}(n) \cosh \kappa_n$. Inserting these states into Eq. (5), we arrive at a recurrence relation for the coefficients C_n for $|n| > 0$,

$$\gamma_n C_n = C_{n-1} + C_{n+1} \quad \text{with } \gamma_n = \frac{2}{\mu} \sqrt{(\epsilon + n\omega)^2 - 4J^2}, \quad (9)$$

where we have defined $C_0 \equiv A \cos \theta$. The solution for this second order recurrence relation is fixed up to an overall constant by requiring convergence for $|n| \rightarrow \infty$ and can be solved efficiently numerically. The angle θ is then given by Eq. (5) for $n = 0$ in terms of those coefficients

$$\tan \theta = \frac{\mu}{2u_k} \left(\frac{C_{-1}}{C_0} - \frac{C_1}{C_0} \right) \quad (10)$$

where we defined $u_k \equiv 2J \sin k$ as the particle velocity.

Since the bound states for $|n| > 0$ do not contribute in the transmission, it is now straight-forward to calculate the transmission coefficient to be

$$T = \cos^2 \theta = \frac{u_k^2}{u_k^2 + (\mu(C_{-1} - C_1)/2C_0)^2}. \quad (11)$$

The transmission obeys $T(\epsilon) = T(-\epsilon)$. For $\epsilon = 0$ the solution becomes symmetric $C_n = C_{-n}$, which results in $T(\epsilon = 0) = 1$ independent of μ for $\omega > \omega_c$ due to Klein tunneling [28]. In the following we assume $\epsilon \neq 0$.

Next we consider lower frequencies $\omega < \omega_c$, when unbound states also exist for $n \neq 0$. In this case it is useful to make an ansatz for an incoming wave at energy ϵ and transmitted/reflected waves in all unbound channels [29]. In this way it is possible to solve for all parameters. Finally, the total transmission coefficient can again be expressed by the solution of the recurrence relation in Eq. (9), which now involves the remaining bound states.

Results.— Using this procedure the exact numerical solution for the transmission coefficient was obtained as shown in Fig. 2 for a given energy $\epsilon = 0.5J$ as a function of μ and ω . Perfect transmission $T \rightarrow 1$ can be

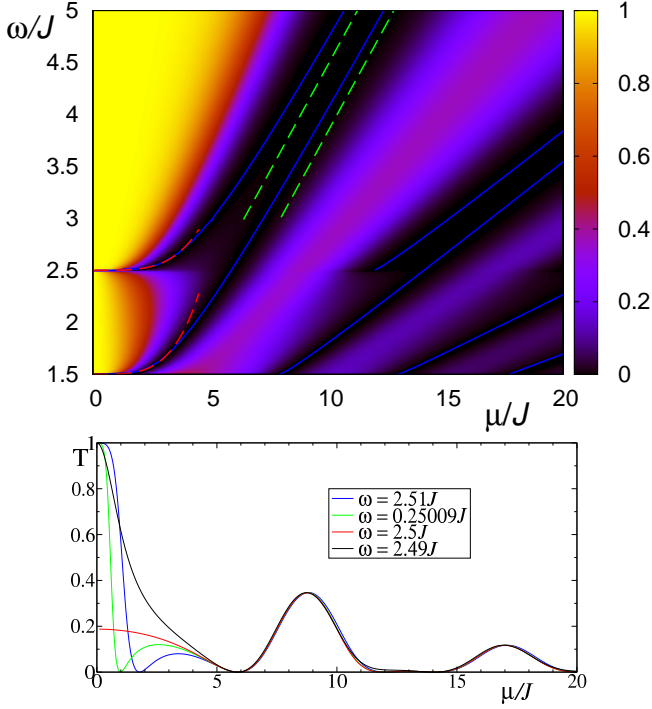


FIG. 2: Exact results for transmission coefficient T as a function of amplitude μ and frequency ω for an incoming wave of energy $\epsilon = 0.5J$. *Top*: The solid lines (blue) indicate the exact values of the resonances ($T = 0$) while the dashed lines are analytical expressions from the first zeros of Bessel functions $J_{\pm\epsilon/\omega}$ in Eq. (13) at large frequencies and the small μ approximations in Eq. (14). *Bottom*: Behavior close to the critical frequency $\omega \approx \omega_c = 2.5J$. For $\omega = \omega_c$ the transmission approaches $T \rightarrow (2J - |\epsilon|)/8J$ as $\mu \rightarrow 0$.

observed for small μ or large frequencies. For increasing μ there is a sharp drop, however, and at special resonances a vanishing transmission $T = 0$ can be observed (blue solid lines). Interestingly, the transmission then increases again with increasing μ before more resonances with $T = 0$ are reached and so on. This apparent non-monotonic behavior with potential μ and frequency ω can be understood in the high frequency limit, where the recurrence relation can be solved analytically. In particular, note that $\gamma_n \rightarrow 2|n\omega + \epsilon|/\mu$ for $\omega \gg J$, so that Eq. (9) becomes exactly the defining recurrence relation for the Bessel functions [30] in this limit. For convergence as $|n| \rightarrow \infty$ the coefficients therefore can be chosen to be Bessel function of the first kind

$$C_n \approx J_{|n+\epsilon/\omega|}(\mu/\omega). \quad (12)$$

The recurrence relation then approaches $C_0 \approx J_{\pm\epsilon/\omega}$ for $n \rightarrow 0^\pm$ from above/below. Accordingly Eq. (10) can be approximated for $\omega \gg J$

$$\tan \theta \approx \frac{\mu}{2u_k} \left(\frac{J_{1-\epsilon/\omega}(\mu/\omega)}{J_{-\epsilon/\omega}(\mu/\omega)} - \frac{J_{1+\epsilon/\omega}(\mu/\omega)}{J_{\epsilon/\omega}(\mu/\omega)} \right). \quad (13)$$

These Bessel functions explain some of the observed fea-

tures of T in Eq. (11), namely the oscillating behavior with μ and ω and resonances of $T = 0$ close to the zeros of the Bessel functions $J_{\pm\epsilon/\omega}$, which are marked in Fig. 2 as dashed lines (green). Moreover, the behavior in Fig. 2 indeed only depends on the ratio μ/ω for large frequencies.

While the description in terms of Bessel functions is useful, this does not explain the behavior in the most interesting region close to $\omega \approx \omega_c$ where the data shows large gradients in the transmission coefficient. In Fig. 2 (bottom) the behavior changes dramatically with frequencies just above or below $\omega_c = 2.5J$ for small driving potential μ . There is a resonance with $T = 0$ which quickly shifts to smaller μ as the frequency is lowered ($\omega = 2.51J$ and $2.5009J$) and suddenly disappears completely once the $n = -1$ chain supports unbound solutions ($\omega = 2.49J$). Exactly at the critical frequency $\omega_c = 2.5J$ the results for $\mu \rightarrow 0$ show a well-behaved finite value $T \rightarrow (2J - |\epsilon|)/8J$, which corresponds to $C_{-1}^2/C_0^2 \rightarrow \gamma_{-2}^2$ and is neither close to unity nor zero. By looking very carefully one observes that there is another resonance close to $\mu \approx 11.5J$ which disappears at ω_c . Away from these singular points the changes of the transmission are very small, however, and appear to be continuous as the frequency goes through the critical value.

Resonances.— It is worth noticing that the resonances $T = \cos^2 \theta = 0$ for $\omega > \omega_c$ are special points at which the coefficient $\phi_{0,0} = C_0 = A \cos \theta$ vanishes exactly. In this case the side coupled systems of the corresponding static problem in Eq. (5) become decoupled from the chain with $n = 0$ in Fig. 1 (left). *Therefore a resonance with $T = 0$ for $\omega > \omega_c$ occurs if and only if the isolated side system has an eigenenergy inside the band $|\epsilon| < 2J$.*

This is a remarkable statement since the decoupled side chains for $n \neq 0$ only support bound states outside the band. However, due to the local coupling μ between the chains one of these energies is pushed inside the band, for which $T(\epsilon) = 0$. Such *Bound States in the Continuum* (BIC) were first proposed by von Neumann and Wigner for a *spatially* oscillating potential in the early days of quantum mechanics [31]. Since then BIC's have received extensive attention in the context of transport phenomena [32–34]. The suppression of transmission is closely related to the Fano-Effect in this case [35, 36].

In order to illustrate the connection with the Fano effect the behavior as a function of incoming energy at fixed frequency $\omega = 3J$ is shown in Fig. 3 (top). The characteristic asymmetric lineshape of Fano resonances is clearly visible. In analogy to the critical frequency in Eq. (7), it is possible to define a critical energy $\epsilon_c = \omega - 2J$, above which the first side chain supports an unbound solution. We observe that a sharp resonance occurs just below this energy for small μ which then broadens and moves quickly away from this point with increasing μ . The lower part of Fig. 3 shows the behavior for larger frequency $\omega = 10J$, where the resonances are further apart

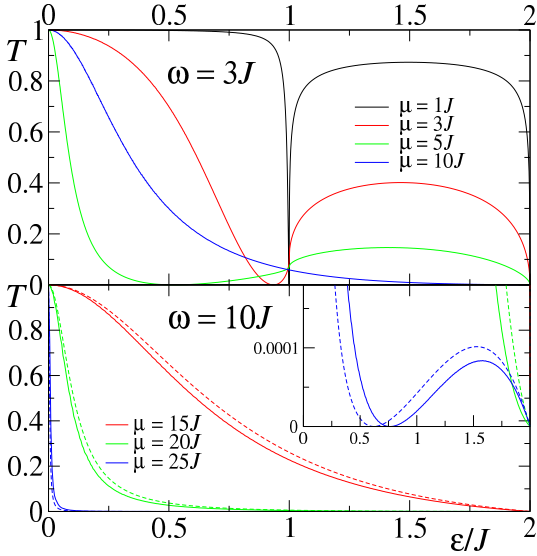


FIG. 3: Transmission coefficient as a function of incoming particle energy ϵ at $\omega = 3J$ (top) and $\omega = 10J$ (bottom). The dashed lines in the bottom plot depict the high frequency approximation in Eq. (13). The inset shows an enlarged region of the resonance for $\mu = 25J$.

and less pronounced (see inset). In this limit the agreement with the high frequency approximation in Eq. (13) fits reasonably well (dashed lines in Fig. 3). The drop of the transmission $T \rightarrow 0$ for $\epsilon \rightarrow 2J$ occurs due to the vanishing of the particle velocity $u_k \rightarrow 0$ and is not connected to any resonance phenomenon.

As shown in Fig. 3 for fixed μ and ω there is at most one energy with $T = 0$ and in some cases it is not possible to find a resonance at all, e.g. for $\omega = 3J$ and $\mu = 10J$. This is in contrast to the situation of a given energy discussed above in Fig. 2 where there are always one or more resonance frequencies for any value of μ .

In order to predict the location of the resonances with $T = 0$ we now follow the strategy to consider the eigenenergies of the decoupled side system in Fig. 1 using Eq. (5) with $\phi_{0,0} = 0$. In fact, the two sides for $n > 0$ and $n < 0$ have identical eigenenergies ϵ , due to the symmetry transformation $\phi_{j,n} \rightarrow (-1)^{n+j} \phi_{j,-n}$. Of course there are infinitely many eigenenergies, but only those inside the band $|\epsilon| < 2J$ are of interest. Let us focus on the resonances $T = 0$ close to the critical frequency $\omega \approx \omega_c$ in the limit of small $\mu \ll J$. In this case, Eq. (9) must still hold for $C_0 = 0$, with $\gamma_{n \neq 1} \gg 1$ and $\gamma_1 \ll 1$. Looking at the first few terms of the recurrence relation it becomes clear that the coefficients grow beyond bounds unless $1 - \gamma_1 \gamma_2 \ll \gamma_1 \ll 1$. Solving for the frequency at which $\gamma_1 \gamma_2 = 1$ we find for the resonance positions

$$\omega \approx \omega_c + \frac{\mu^4}{64J([4J - \epsilon]^2 - 4J^2)}, \quad (14)$$

which is marked by dashed lines (red) in Fig. 2 and agrees

well with the exact results. Using the condition $\gamma_1 \gamma_2 = 1$, resonances can also be found at fixed ω for small deviations from the critical energy ϵ_c , which are again proportional to μ^4 .

Conclusions.— In summary we have developed a framework to study the transmission across an AC driven barrier connected to leads of finite bandwidth based on the Floquet formalism. The resulting transmission coefficient T can be calculated exactly and shows versatile tunability with frequency ω , energy ϵ , and impurity strength μ . At high frequencies $\omega \gg J$ the transmission can be expressed in terms of Bessel functions, which also appear in the description of so-called coherent destruction of tunneling. In this limit the oscillations can be averaged to form an effective quasi-static hopping $J_{\text{eff}} = JJ_0(\mu/\omega)$ [4, 37]. In our case, a slightly more refined picture emerges in terms of Bessel functions with a fractional index $\nu = |n| \pm \epsilon/\omega$.

However, much more interesting effects appear at lower frequencies $\omega \approx \omega_c = 2J + |\epsilon|$ where there are sharp changes in T and a complete breakdown of the transmission $T = 0$ may appear even for arbitrarily small barriers μ . The explanation of such a *quantum resonance catastrophe* can be found in the dynamically created side coupled chains in Fig. 1, which contain bound states for all energies *outside* the band for $\omega > \omega_c$. The effect of the local coupling μ between the chains is to push one energy from just above the band into the continuum. Thus effectively a discrete *Bound State in the Continuum* is formed, which is known to have drastic effects on the transmission [31] based on the Fano effect [35]. There has been an interesting proposal to use static side coupled systems to engineer Fano resonances [36], but the creation of “virtual” side coupled systems by AC driving considered here is even simpler and more versatile than any static design. The location of the resulting resonances for $\mu \rightarrow 0$ can be predicted rather accurately by Eq. (14). It should be noted that the width of the resonance also changes dramatically near ω_c . While this may become the limiting factor to observe the quantum resonance catastrophe for very small μ , it also presents a unique opportunity for the design of switches, where a huge change of transmission for small parameter changes near sharp resonances is a desirable feature.

The underlying tight-binding model has long been used in condensed matter, but with the recent trend of designing tailored quantum systems, this model has made a revival for the realistic description of corresponding setups in molecular electronics, quantum nano dots, and photonic materials. For ultracold gases in optical lattices [21] it is now possible to insert localized impurities [22], which play the role of a local barrier that can easily be periodically changed using Feshbach resonances. Given the large variety of applicable systems it is difficult to anticipate which experimental realization is best suited to explore the quantum resonance catastrophe predicted

here.

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